Q&A - Lecture 2

Is there a relation between compatible and incompatible variables? For example, because spin and position are compatible and position and velocity are incompatible, is there a relation that we can derive for spin and velocity ?

There is no relation of the type that you propose between incompatible observables. There is, however, a relationship between incompatible observables like momenta and coordinates and this is the Heisenberg uncertainty principle. This can be generalized to a relationship between two operators that do not commute and a relationship between the uncertainties in their measurements.

If the action of an operator on an arbitrary state is defined as a sum of eigenkets multiplied by coefficients and their eigenvalues, why can a measurement only take a specific eigenvalue and not a combination of eigenvalues?

This is one of the core postulates of quantum mechanics, validated by experiments. Not sure I can say much more about it…but let me know if you wish to discuss it further!

When talking about the phase space, there was no mention of ergodicity. Is ergodicity not relevant in this conversation or is it such an unrealistic approximation that we don't make use of it?

Ergodicity is actually crucial in the conversation. In fact, the correspondence between the points visited by a trajectory in time and the (stationary, in our case equilibrium) probability in phase space requires it.This was one of the things I was referring to (though I did not say it specifically) when I mentioned that the derivation I was outlining has several mathematically delicate aspects. I would not call ergodicity an approximation but rather an hypothesis. And, though it is a very difficult property to prove (to the best of my knowledge this has been done for very few classical systems such as the hard spheres), I would not call it unrealistic: numerical experiments actually seem to verify for interacting systems in different ensembles “almost” always.

In quantum mechanics, measurements are inherently random, but simulations rely on pseudorandom number generators, which are deterministic. How do simulations accurately capture the true randomness of quantum systems using pseudorandom numbers? Are there any limitations or significant differences when using pseudorandom numbers instead of true randomness?

Let me be fussy: in quantum mechanics the measurement - being the calculation of the action of operators on states is not random. Also, the evolution of a quantum state via the time-dependent Schrödinger equation is completely deterministic. Probability comes in the interpretation of the results of measurements. The use of pseudorandom numbers is essentially inevitable - unless one wants to go via very roundabout ways - and need to be accounte for both in classical and in quantum simulaitons. There are a number of highly sophisticated pseudorandom number generators that can pass many tests on correlation between successive extractions and periodicity of extraction. When these tests - always a good idea to perform some when adopting an untested pseudorandom number generator - are passed, there are no significant differences with fully random simulations and no effect on results.

In the SOFT algorithm, I have the impression that we're trying to find out the cinetic energy and the potential energy at the same time, but wouldn't that be impossible (as these two observables are not compatible)?

Is the 6th postulate telling us that when when doing a measurement or a system and putting it in an eigenstate, we're supposed to obtain the same eigenvalue if we measure the same observable immediately, without letting the time-evolution propagate? If it is the case, is an "immediate"measurent feasible on such time-scale? »

Not sure about the numbering but…yes, there is such a postulate and nice question. If the observable is the Hamiltonian, then the state will not change anymore. If the observable commutes with the Hamiltonian, I'd say the same. If the observable does not commute with the Hamiltonian…instantaneous refers to the typical time-scale of evolution. I think that this can be made more precise via a variation on the theme of the so-called adiabatic theorem.

As you introduced in class, the time evolution can be written as the exp(-i H/hbar t) \ket{\psi(0)}. If we write the Hamiltonian as a matrix and the quantum state as a vector. We can directly implement matrix exponential of H in MATLAB and directly compute the time evolution of the quantum system by implementing the matrix onto the quantum state vector. Is this idea applicable? I guess not but I am confusing why it doesn't work.

The procedure you describe works. However, the cost of the operations in it is still exponential — unless approximations are performed. Edrick and Federica will upload a paper with different ones.

Under Heisenberg's Uncertainty Principle, we know that momentum and position of a quantum particle cannot be simultaneously measured. However, the Hamiltonian *operator for the time evolution of a quantum system includes kinetic and potential terms which have both position and momentum components. Is this not contradictory, or are we relying on certain approximations to allow for this?*

No contradiction: The Hamiltonian - i.e. the operator associated to the energy - is a separate observable and admits a set of eigenvalues and eigenvectors that are not (except in trivial cases) those of the momentum and the coordinates. The non-commutativity of momenta and coordinates means that we cannot find a basis that will give us simultaneously the eigenvalues of the momentum and those of the coordinate. This is respected, for example, when using the SOFT algorithm to propagate, since there we have to go via a change of basis when looking at the action of the kinetic and potential terms exponential of the Hamiltonian (after Trotter).

What order of magnitude can current computer handle in terms of number of parameters ?

I don’t know the “absolute numbers”. If we frame this in the context of class - i.e. computer simulations of quantum systems, based on methods that exploit the capabilities for classical systems - then relevant numbers are

1. For generic interacting classical systems, millions of degrees of freedom can be propagated for times in the range of microsconds (milliseconds on dedicated architectures)

2. For generic interacting quantum systems, tenths of degrees of freedom can be propagated for times in the range of picoseconds.

What happens if we have 2 interacting systems? Is there a way to compute our parameters? Find the equation of evolution?

Not sure to understand the question. If we have the interaction potential between the two systems (as is the case in classical molecular dynamics) then yes, we can find the evolution equations and integrate them using Verlet. What do you mean by compute our parameters? The parameters of the potential or something else?

The question that I had about the course is more about mathematics. You said during class that the state vector at any time can be described by an operator (an exponential containing a constant, time and the Hamiltonian) acting on the initial value of the state vector at t=0. I’m not sure that I understand where this comes from (the exponential term). Is there any mathematical proof of it, or a conceptual way that you could explain it to me ?

Mathematically, the statement can be proven by verifying that the evolved state satisfies the (abstract) time-dependent Schrödinger equation. This can be done by simply considering the left and right sides, with the state at t expressed as the exponential of the operator (times the appropriate constants) and taking the derivative with respect to the parameter t. In doing so, keep in mind that the Hamiltonian operator commutes with any function of the Hamiltonian operator.

In the lecture we discussed coordinate discretisation to numerically solve the evolution of a quantum state. Discretization implies that coordinates must be bounded from below and above. Does this mean that we can only solve evolution for localised wavefunctions?

The wavefunction (i.e. the coefficients of the state in the coordinate representation), must be L_2 - in other words square integrable on the x axis (this comes from the interpretation of the modulus square of the wavefunction as a probability density). This implies that bounding is possible. Of course, if the wavefunction is very delocalises, we need a wide interval and - most likely - many grid points.

Concerning the Trotter break-up; is this method necessary because the operators K and V don’t commute? Furthermore, do we use a fourier transform in the SOFT for the same reason (position and momenta operators don’t commute)?

Exacly, we need Trotter to express the exponential of the sum of the non-commuting operators into the product of the exponential.
Indirectly: we have to change basis to evaluate the potential and kinetic parts of the propagation because the operators do not commute. The transformation corresponding to this basis change can be implemented using fourier transforms.

During the lecture, we expanded the state vector as a linear combination of eigenvector of a given operator. Is this the only way to find a basis for this, or is there any other meaningful basis to expand the state vector in ?

Any valid (i.e. compatible with the Hilbert space of the system) basis is admissible. In fact, the choice of basis is a freedom that can be exploited - as done, for example, in the SOFT algorithm - to enable or simplify the evaluation of matematical expressions. Eigenvectors are the optimal choice for a GIVEN operator.

When one performs measurement on a system (mathematically), the state of the system changes to the corresponding eigenstate. What does it physically mean, will the system really change its behavior in a physically observable way ? Can we measure physically a specific state of a system, or only averages ?

Yes: if we repeat the measurement of an observable after having found one of its eigenvalues, the system will CERTAINLY be in the corresponding eigenstate; Here one needs to be careful. Strictly speaking, the state of the system is not an observable: only the values of observables as expressed by eigenvalues (not eigenstates) of operators can be measured. When the state is expressed as a linear combination (with many non-zero coefficients) in a given basis, mathematically, we have access to averages.

Why do we use Trotter's formula instead of Baker–Campbell–Hausdorff's formula?

A matter of compromizing between accuracy and numerical cost of the approximation. Adding commutator terms in the exponential product requires to evaluate them and this can lead to operators (e.g. derivatives of the potential) that are expensive to compute. That said, sometimes, higher order formulas like BCH are indeed used. Not in SOFT, though.

What are the differences of |ψ>, ψ, and |ω>? Is a wave function different from a vector?

We have indicated with |ψ> a generic state of the system, while |ω> was reserved for the eigenvector of operator capital Omega (hat) with eigenvalue ω. Not sure where I used the symbol ψ alone,can you give me an example? If you mean ψ(x), i.e. a wave function, then this leads me to your sedon question

Is a wave function different from a vector?

Yes! The wave function is the coefficient of the expansion of a state vector in the coordinate basis. I'll say more about this in the next class.

If we want to numerically solve the Schrödinger equation for the wave function, we discretize the x axis and solve the Schrödinger equation for each segment. In that case should we also discretize the kinetic and potential and energy of the Hamiltonian, how do we do it for the kinetic energy ?

We solve for each grid point on the x axis. For the kinetic part, we use the change of basis from x to p to move to the p axis (via the fourier transform) and then evaluate the exponential of the kinetic energy at each p grid point. Then we use an inverse fourier transform to go back to the x basis for the following evaluation of the exponential of the potential.

"What is the'dt' time you have mentioned in your course for a quantum measurement? 1 ms? 1s? Does it depend on the observable we measure?

was the dt in connection with a generic measurement or in connection to the time-evolution? In the latter case, typical dt is fractions of fs.

What would be a conceptual or qualitative definition of the quantum average ? How does it differ from the definition of the classical average ?

The quantum average is defined for each quantum state as the action of the operator on the state projected on the same (original) state. It gives a weigthed average of the eigenvalues of the operator, where the weight - that has the probabilistic interpretation that you mention in the summary - is the probability to find the system in the eigenstate of the operator. It is intrinsecally different from a classical average - as introduced in class - because we cannot interpret the results of microscopic experiments without it. For the classical average, the microscopic result of an experiment is well defined, but we need averages to connect to macroscopic measures.

In the SOFF algorithm, I have the impression that we're trying to find out the cinetic energy and the potential energy at the same time, but wouldn't that be impossible (as these two observables are not compatible)?

We are not finding out these observables at the same time. We are evaluating in sequence the action of each of them on the “original state”. Note that this is done b,. e.g., first evaluating the action of the exponential of the potential in the coordinate basis. This changes the state by changing its coefficients. Then we change basis - the need to do so is a manifestation of the incompatibility of the observables - to the momentum basis and we evaluate the action of the exponential of the kinetic operator on the TRANSFORMED state. If we had applied the operators in reverse order the result would not have been the same — in SOFT the difference is order dt^2 or dt^3…This is, again, a manifestation of the incompatibility.